Mathematical Model for a Fuel Cell Cathode

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A new phenomenological mathematical model that describes the behavior of the cathode of a polymeric fuel cell was developed. It includes the modelling of liquid water and all cathode layers (gas collector, gas diffusion layer, microporous layer and catalyst layer); additionally, the catalyst layer is described as spherical agglomerates according to experimental evidence [1].

Since the performance of the fuel cell is highly dependent on the structure of the catalyst; [2] and cell flooding cause decrease in oxygen transport and loss of active catalyst surface [3] affecting fuel cell efficiency. The model considers these two important aspects in order to obtain a better description of the phenomena.

As a purely predictive model, it only requires the design specifications of the membrane electrolyte assembly (MEA). Once the data is provided (thickness of the catalyst layer, the catalyst load, the fraction by weight of platinum on carbon, the weight fraction of ionomer inside the catalyst layer and the ionomer density) all other model parameters are derived through the balance equations.

The model solution provides the current density, the cell potential, ethanol crossover rate and concentrations in the catalytic layer and in the membrane. It can be used to calculate and predict fuel cell behavior with high accuracy.

It takes into account liquid saturation in the pores and apply the spherical agglomeration method for describing the topology of the catalytic layer. The two-phase method is used for the macroscopic description of the system, resulting in a differential model, which is solved by the Runge-Kutta Fehlberg method with prediction and correction of error.

References

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